

Ab initio method for examining the halo structure of ${}^6\text{He}$. I. Coordinate space two-nucleon correlations

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We evaluate pairwise correlations using full ground state wave functions for ${}^4\text{He}$ and ${}^6\text{He}$ obtained by *ab initio* configuration interaction methods with the Daejeon16 nucleon-nucleon interaction, to characterize the structures of these two systems. We show that the two-nucleon spatial correlations $f(r^n)$, for instance, the pair-identity operator r^0 and the square-separation operator r^2 , can shed light on the halo structure of ${}^6\text{He}$ relative to ${}^4\text{He}$. To the best of our knowledge, this is the first attempt of examining the nuclear structure directly using two-body spatial correlations projecting on two-body total quantum numbers (such as the two-body total spin S) with the no-core shell model (NCSM). Connecting the expectation values of r^0 for ${}^6\text{He}$ with those for ${}^4\text{He}$, we conclude that the two valence neutrons in ${}^6\text{He}$ dominantly form a spin-singlet configuration when the symmetry regarding the probability of forming an arbitrary two-body total spin is respected. The root-mean-square separation between two nucleons for each projecting sector is calculated using the expectation value of r^2 combined with r^0 . For completeness, even without fully convergent results, we compare the point-nucleon root-mean-square radii calculated from r^2 with those obtained from experiments.

I. INTRODUCTION

Clustering phenomena in atomic nuclei reflect both the degrees of freedom of individual nucleons and collective structures within the nucleus. As a natural example, certain nuclei near the “drip lines” (where nucleons are nearly free to escape) form a more tightly bound core and a “halo” made of one or more nucleons loosely bound to the core [1–5].

Neutron halos have drawn significant attention since the 1980s when the surprisingly large interaction cross section of ${}^{11}\text{Li}$ compared with other Li isotopes was observed in radioactive ion beam (RIB) transmission experiments [6–8]. They also display a narrow core momentum distribution in peripheral breakup reactions [9, 10]. Strong electric dipole ($E1$) excitations at low excitation energies were observed in some of the halo nuclei, attributed to their weakly bound halo neutron(s) undergoing excitation to the continuum states [11–13]. Although there is no clear-cut distinction between the halo and non-halo nuclei, halo nuclei are recognized by their shared characteristics. Nuclei with a neutron halo, for example, display a long tail in the neutron density distribution profile, and have small neutron separation energies for the halo neutron(s).

Over the years, many efforts have been made to extract the clustering information from *ab initio* calculations. The *ab initio* NCSM/RGM (no-core shell model/resonating group method) was used to perform calculations on a ${}^4\text{He}$ (g.s.) + $n + n$ cluster basis which was consistent with *ab initio* NCSM calculations without a cluster basis [14–16]. Cluster form factors were ex-

tracted [17], and further improvements have been made to the work on three-cluster dynamics within the *ab initio* NCSM with continuum [16, 18]. The *ab initio* lattice approach implementing chiral effective field theory successfully modeled a 3- α structure for the Hoyle state of ${}^{12}\text{C}$ [19]. More recently, *ab initio* configuration interaction methods have revealed important roles of α -clustering in light nuclei including details on the ground and Hoyle excited state of ${}^{12}\text{C}$ [20]. In addition, measures of entanglement of ${}^4\text{He}$ and ${}^6\text{He}$ nuclei were explored using *ab initio* nuclear many-body calculations [21], where a core-valence structure naturally emerges from the full no-core calculation of ${}^6\text{He}$ by analyzing common features of entanglement.

From a computational point of view, studying the clustering properties of nuclei could help us design improved basis functions and to usefully subdivide the Hilbert space into regions of greater and lesser importance. Spatial information such as the average relative separations of nucleons in a system is key to characterizing the cluster wave functions.

Thus, we examine the structure of a nucleus by *ab initio* calculations, utilizing two-body correlations. Previously, one-body probabilities have been used in the *ab initio* NCSM [22] with great success in revealing information on the clustering of Li isotopes [23, 24] and ${}^9\text{Be}$ [24], a one-neutron halo nucleus. Using two-body operators has the advantage of unfolding the detailed structure of the dominant configuration and displaying the differences in the nucleon-nucleon correlations among pairs of nucleons in specific two-body states.

We choose ${}^6\text{He}$ as a test case for this new method ow-

ing to its relative simplicity. It is the lightest Borromean halo nucleus which means that none of the available two-component substructures (n - n or n - α in the $\alpha+n+n$ system) are bound when one removes any third component. In this case, the one-body density profile cannot fully reveal the geometrical structure for the $2n$ -halo, while two-body correlations can probe the relative distance between the two valence neutrons compared with the relative distances of the other pairs of nucleons. Our primary focus is to introduce our method and demonstrate its application to ${}^6\text{He}$ in advance of achieving fully converged *ab initio* NCSM results for the two-body correlations that we develop and employ. We defer the development of suitable extrapolation methods for these two-body correlations to a later project.

In the following sections, we first introduce the coordinate space two-body operators we will use (Sec. II) and the approach to solving the quantum many-body problem (Sec. III). We then present and discuss the calculated expectation values of these two-body operators and how they relate to the halo structure of ${}^6\text{He}$ (Sec. IV).

II. CONSTRUCTING TWO-BODY OPERATORS IN COUPLED- J BASIS

In order to carry out a quantitative analysis of the distributions of nucleons and pairs of nucleons within a nucleus, one needs appropriate operators that sample these quantities. For this purpose, we will define one-body and two-body operators whose expectation values within the nuclear ground state will inform our detailed analysis of how nucleons are arranged in coordinate space on average. From this arrangement, we hope to infer if a halo structure is emerging from the quantum many-body wave functions.

A. One- and two-body operators in the occupation representation

One-body operators are defined as [25]

$$\mathcal{O}_{1\text{B}} = \sum_{\alpha,\beta} O_{\alpha\beta} a_{\alpha}^{\dagger} a_{\beta}, \quad (1)$$

where

$$O_{\alpha\beta} = \langle \alpha | \mathcal{O} | \beta \rangle \quad (2)$$

are the one-body matrix elements and the Greek subscripts label the single-particle states in an ordered sequence. The single-particle states are related to creation operators acting on the vacuum,

$$|\alpha\rangle = a_{\alpha}^{\dagger} |0\rangle. \quad (3)$$

Similarly, two-body operators are defined as [25]

$$\mathcal{O}_{2\text{B}} = \sum_{\alpha < \beta, \gamma < \delta} O_{\alpha\beta\gamma\delta} a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_{\delta} a_{\gamma}, \quad (4)$$

where

$$O_{\alpha\beta\gamma\delta} = \langle \alpha\beta | \mathcal{O} | \gamma\delta \rangle = \langle 0 | a_{\beta} a_{\alpha} \mathcal{O} a_{\gamma}^{\dagger} a_{\delta}^{\dagger} | 0 \rangle \quad (5)$$

are the two-body matrix elements. Due to the fermion anticommutation relation $a_{\alpha}^{\dagger} a_{\beta}^{\dagger} = -a_{\beta}^{\dagger} a_{\alpha}^{\dagger}$, the two-body matrix elements are antisymmetric under interchange of each pair of two-body state labels.

Let us now focus only on the two-body operators. The expectation value of a two-body operator between an initial state $|\Phi_A\rangle$ and a final state $|\Phi'_A\rangle$ in a system of nucleons is thus

$$\langle \Phi'_A | \mathcal{O}_{2\text{B}} | \Phi_A \rangle = \sum_{\alpha\beta\gamma\delta} \rho_{\alpha\beta\gamma\delta} \langle \alpha\beta | \mathcal{O} | \gamma\delta \rangle, \quad (6)$$

where $\alpha < \beta, \gamma < \delta$ is implicitly assumed wherever summing pairs of two-body state labels, and

$$\rho_{\alpha\beta\gamma\delta} = \langle \Phi'_A | a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_{\delta} a_{\gamma} | \Phi_A \rangle \quad (7)$$

defines matrix elements of the two-body density matrix.

B. Two-body operators in the coupled- J basis

The standard basis we use is the single particle basis, which is denoted by its quantum numbers including radial quantum number n , orbital angular momentum l , spin s , total angular momentum j , total angular momentum projection m_j , isospin t and isospin projection t_z . We can use the short-hand notation

$$\alpha = \{n_{\alpha}, l_{\alpha}, \frac{1}{2}, j_{\alpha}, m_{j_{\alpha}}, \frac{1}{2}, t_{z\alpha}\}, \quad (8)$$

where the first “ $1/2$ ” is for nucleon spin s and the second “ $1/2$ ” is for nucleon isospin t .

To compute matrix elements of two-body operators in a basis with “good” angular momentum, two-body total angular momentum J , we work in terms of the spherical tensor coupled product [26], e.g.,

$$\{a_{\alpha}^{\dagger} a_{\beta}^{\dagger}\}_{J,M} = \sum_{m_{j_{\alpha}}, m_{j_{\beta}}} C_{m_{j_{\alpha}} m_{j_{\beta}} M}^{j_{\alpha} j_{\beta} J} a_{\alpha}^{\dagger} a_{\beta}^{\dagger}, \quad (9)$$

where M is the z -projection of the two-body total angular momentum. $C_{m_{j_{\alpha}} m_{j_{\beta}} M}^{j_{\alpha} j_{\beta} J}$ are the Clebsch-Gordan coefficients. The transformed coupled basis is called coupled- J basis. The resulting coupled- J basis states are

$$|\alpha\beta; J\rangle = \{a_{\alpha}^{\dagger} a_{\beta}^{\dagger}\}_{J} |0\rangle. \quad (10)$$

When one aims to calculate only observables represented by one-body and two-body operators, one may simply compute the one-body and two-body density matrices between the desired initial and final states, and the matrix elements of all one-body and two-body operators may subsequently be extracted from the weighted sum of these density matrices.

153 The two-body density matrix in the coupled- J basis,
154 suppressing M for compactness of notation, is

$$\begin{aligned} \rho_{\{\alpha\beta\},J',\{\gamma\delta\},J} &= \langle \Phi'_A | \{a_\alpha^\dagger a_\beta^\dagger\}_{J'} \{a_\delta a_\gamma\}_J | \Phi_A \rangle \\ &= \sum_{m_{j_\alpha}, m_{j_\beta}} C_{m_{j_\alpha} m_{j_\beta}}^{j_\alpha j_\beta J'} \sum_{m_{j_\gamma}, m_{j_\delta}} C_{m_{j_\gamma} m_{j_\delta}}^{j_\gamma j_\delta J} \rho_{\alpha\beta\gamma\delta}. \end{aligned} \quad (11)$$

155 The expectation value of a two-body operator in a sys-
156 tem of nucleons expressed in the coupled- J basis can thus
157 be written as

$$\langle \Phi_{A'} | \mathcal{O}_{2B} | \Phi_A \rangle = \sum_{\{\alpha\beta\},J',\{\gamma\delta\},J} \rho_{\{\alpha\beta\},J',\{\gamma\delta\},J} \langle \alpha\beta; J' | \mathcal{O} | \gamma\delta; J \rangle, \quad (12)$$

158 where \mathcal{O} is redefined as an operator acting on the
159 coupled- J basis.

160 C. Rotationally invariant operator with given 161 two-body total spin and given pair of isospin 162 projections

163 We consider matrix elements of local two-body op-
164 erators of the form $O(r)P_S$, that is, a rotationally in-
165 variant (scalar) operator depending only on the relative

166 spatial coordinate r of the two nucleons, in combina-
167 tion with the two-body total spin projection operator P_S ,
168 where $\langle S_1 | P_S | S_2 \rangle = \delta_{S S_1} \delta_{S S_2}$. We adopt the shorthand
169 $\mathcal{O}(r)[S] \equiv O(r)P_S$, and below we will focus on opera-
170 tors $\mathcal{O}(r)[S, t_{za}, t_{zb}]$ which also project on given isospin
171 projections t_{za} and t_{zb} of the two nucleons.

172 Since the $O(r)$ operator is a rank-0 tensor, from
173 the Wigner-Eckart theorem, $\langle \alpha\beta; J' M' | O(r) | \gamma\delta; J M \rangle =$
174 $\delta_{J' J} \delta_{M' M} \langle \alpha\beta; J | | O(r) | | \gamma\delta; J \rangle$, where, in our convention,
175 the double-bar (reduced) matrix element does not factor
176 out $(2J+1)^{-\frac{1}{2}}$ and remains consistent with the Wigner-
177 Eckart theorem formulated in Eq. (4.15) of Ref. [27].

178 In order to select the states of given two-body total
179 spin, one can resolve quantities in terms of two-body total
180 spin S ($\vec{S} = \vec{s}_\alpha + \vec{s}_\beta$) and two-body total orbital angular
181 momentum L ($\vec{L} = \vec{l}_\alpha + \vec{l}_\beta$) by inserting

$$\mathbb{1} = \sum_{LS} |n_\alpha l_\alpha n_\beta l_\beta L, \frac{1}{2} \frac{1}{2} S; J\rangle \langle n_\alpha l_\alpha n_\beta l_\beta L, \frac{1}{2} \frac{1}{2} S; J| \quad (13)$$

182 twice, where the spin quantum numbers ($\frac{1}{2}$) are explicit
183 while the isospin quantum numbers are omitted for sim-
184 plication of the notation.

185 We find that the reduced matrix element of $\mathcal{O}(r)[S]$
186 can be expressed as

$$\begin{aligned} &\langle \alpha\beta; J | | \mathcal{O}(r) [S] | | \gamma\delta; J \rangle \\ &= \sum_{L_1 L_2 S_1 S_2} \langle \alpha\beta; J | n_\alpha l_\alpha n_\beta l_\beta L_1, \frac{1}{2} \frac{1}{2} S_1; J \rangle \langle n_\alpha l_\alpha n_\beta l_\beta L_1, \frac{1}{2} \frac{1}{2} S_1; J | | O(r) | | n_\gamma l_\gamma n_\delta l_\delta L_2, \frac{1}{2} \frac{1}{2} S_2; J \rangle \langle n_\gamma l_\gamma n_\delta l_\delta L_2, \frac{1}{2} \frac{1}{2} S_2; J | \gamma\delta; J \rangle \\ &\quad \times \delta_{S S_1} \delta_{S_1 S_2} \\ &= \sum_L \langle n_\alpha l_\alpha n_\beta l_\beta L | | O(r) | | n_\gamma l_\gamma n_\delta l_\delta L \rangle \langle \alpha\beta; J | n_\alpha l_\alpha n_\beta l_\beta L, \frac{1}{2} \frac{1}{2} S; J \rangle \langle n_\gamma l_\gamma n_\delta l_\delta L, \frac{1}{2} \frac{1}{2} S; J | \gamma\delta; J \rangle, \end{aligned} \quad (14)$$

187 where in the last line we have used the fact that $O(r)$ is
188 rotationally invariant so the two-body total orbital angu-
189 lar momentum is invariant upon the action of $O(r)$, i.e.
190 $\langle L_1 | O(r) | L_2 \rangle = \langle L_1 | O(r) \delta_{L_1 L_2} | L_2 \rangle$. And we now drop
191 the subscript of L for notational simplicity. There is no
192 need to label J values in the reduced matrix elements,
193 because $O(r)$ only produces a dependence on the radial
194 and orbital quantum numbers.

198 by first expanding the notation

$$\begin{aligned} &\langle \alpha\beta; J | n_\alpha l_\alpha n_\beta l_\beta L, \frac{1}{2} \frac{1}{2} S; J \rangle \\ &= \langle n_\alpha l_\alpha \frac{1}{2} j_\alpha, n_\beta l_\beta \frac{1}{2} j_\beta; J | n_\alpha l_\alpha n_\beta l_\beta L, \frac{1}{2} \frac{1}{2} S; J \rangle \\ &= \langle l_\alpha \frac{1}{2} j_\alpha, l_\beta \frac{1}{2} j_\beta; J | l_\alpha l_\beta L, \frac{1}{2} \frac{1}{2} S; J \rangle \\ &= \sqrt{(2j_\alpha + 1)(2j_\beta + 1)(2L + 1)(2S + 1)} \begin{Bmatrix} l_\alpha & l_\beta & L \\ 1/2 & 1/2 & S \\ j_\alpha & j_\beta & J \end{Bmatrix}, \end{aligned} \quad (15)$$

195 We identify the “ $LS - jj$ ” coupling coefficient [26,
196 28], i.e., the transformation coefficient between Russell-
197 Saunders coupling and the spin-orbit coupling in Eq. (14)

199 where the curly brackets represent the $9j$ symbols, which
200 is another way to write an assembly of Clebsch-Gordan
201 coefficients.

202 One then obtains

$$\begin{aligned}
\langle \alpha\beta; J || \mathcal{O}(r) [S] || \gamma\delta; J \rangle &= \langle n_\alpha l_\alpha n_\beta l_\beta L || \mathcal{O}(r) || n_\gamma l_\gamma n_\delta l_\delta L \rangle \\
&\times (2S+1) \sqrt{(2j_\alpha+1)(2j_\beta+1)(2j_\gamma+1)(2j_\delta+1)} \sum_L (2L+1) \begin{Bmatrix} l_\alpha & l_\beta & L \\ 1/2 & 1/2 & S \\ j_\alpha & j_\beta & J \end{Bmatrix} \begin{Bmatrix} l_\gamma & l_\delta & L \\ 1/2 & 1/2 & S \\ j_\gamma & j_\delta & J \end{Bmatrix}.
\end{aligned} \tag{16}$$

203 To apply this operator on a fixed pair of isospin z -projection values for two nucleons, we define $\mathcal{O}(r)[S, t_{za}, t_{zb}] =$
204 $\mathcal{O}(r) P_S P_{t_{za}, t_{zb}}$, with

$$\begin{aligned}
\langle \alpha\beta; J || \mathcal{O}(r) [S, t_{za}, t_{zb}] || \gamma\delta; J \rangle &= \langle \alpha\beta; J || \mathcal{O}(r) [S, t_{za}, t_{zb}] \delta_{t_{z\alpha}, t_{z\gamma}} \delta_{t_{z\beta}, t_{z\delta}} || \gamma\delta; J \rangle \\
&= \langle \alpha\beta; J || \mathcal{O}(r) [S] || \gamma\delta; J \rangle \delta_{t_{z\alpha}, t_{z\gamma}} \delta_{t_{z\beta}, t_{z\delta}} [\delta_{t_{z\alpha}, t_{za}} \delta_{t_{z\beta}, t_{zb}} + (1 - \delta_{t_{za}, t_{zb}}) \delta_{t_{z\alpha}, t_{zb}} \delta_{t_{z\beta}, t_{za}}],
\end{aligned} \tag{17}$$

205 where the factor $(1 - \delta_{t_{za}, t_{zb}})$ preserves the normalization when $t_{za} = t_{zb}$.

206 The resulting matrix element becomes

$$\begin{aligned}
\langle \alpha\beta; J' M' | \mathcal{O}(r) [S, t_{za}, t_{zb}] | \gamma\delta; J M \rangle &= [\delta_{t_{z\alpha}, t_{za}} \delta_{t_{z\beta}, t_{zb}} + (1 - \delta_{t_{za}, t_{zb}}) \delta_{t_{z\alpha}, t_{zb}} \delta_{t_{z\beta}, t_{za}}] \delta_{t_{z\alpha}, t_{z\gamma}} \delta_{t_{z\beta}, t_{z\delta}} \delta_{J' J} \delta_{M' M} \\
&\times (2S+1) \sqrt{(2j_\alpha+1)(2j_\beta+1)(2j_\gamma+1)(2j_\delta+1)} \\
&\times \sum_L (2L+1) \begin{Bmatrix} l_\alpha & l_\beta & L \\ 1/2 & 1/2 & S \\ j_\alpha & j_\beta & J \end{Bmatrix} \begin{Bmatrix} l_\gamma & l_\delta & L \\ 1/2 & 1/2 & S \\ j_\gamma & j_\delta & J \end{Bmatrix} \langle n_\alpha l_\alpha n_\beta l_\beta L || \mathcal{O}(r) || n_\gamma l_\gamma n_\delta l_\delta L \rangle.
\end{aligned} \tag{18}$$

207 We then introduce a notation to describe an opera- 231 of nucleons with a given two-body total spin S , which will
208 tor acting within a system of nucleons, similar to the 232 be illustrated in Sec. IV B.
209 $U[u]$ and $V[v]$ operators defined in Ref. [29]. The sub-
210 script A of a two-body operator means to apply the oper-
211 ator on all nucleon pairs in the A -body space, $(\mathcal{O}_{2B})_A \equiv$ 233
212 $\sum_{i<j}^A \mathcal{O}_{2B}$. Similarly, the subscript A of a one-body op-
213 erator means to apply the operator on all A nucleons,
214 $(\mathcal{O}_{1B})_A \equiv \sum_i^A \mathcal{O}_{1B}$. Thus, the expectation value of
215 $\mathcal{O}(r)_A[S, t_{za}, t_{zb}]$ is

$$\begin{aligned}
\langle \mathcal{O}(r)_A[S, t_{za}, t_{zb}] \rangle &= \langle \sum_{i<j}^A \mathcal{O}(r_{ij})[S, t_{za}, t_{zb}] \rangle \\
&= \sum_{\text{all } q\#} \sum_{i<j}^A ij \langle \alpha\beta; J' M' | \mathcal{O}(r)[S, t_{za}, t_{zb}] | \gamma\delta; J M \rangle_{ij},
\end{aligned} \tag{19}$$

216 where $r_{ij} = |\vec{r}_i - \vec{r}_j|$ is the relative distance between
217 the i th and j th nucleon, and $i, j = 1, 2, \dots, A$. α and
218 γ (β and δ) denote the initial and final single particle
219 states of the i th (j th) nucleon, respectively. The overall
220 summation runs over all quantum numbers (“all $q\#$ ”).
221 In the following, the subscript A is conveniently omitted
222 when referring to the expectation values of the operator
223 (denoted by a bracket directly around the operator), i.e.,
224 $\langle \mathcal{O} \rangle \equiv \langle \mathcal{O}_A \rangle$.

225 In Sec. IID and Sec. IIE, we will define the pair-
226 identity operator and the square-separation operator
227 in given S and isospin projection pair (proton-proton,
228 neutron-proton and neutron-neutron, indicated as pp , pn ,
229 and nn) sectors. Combining them will give us the infor-
230 mation on mean square separations of a pp , pn or nn pair

D. Pair-identity operator

234 The pair-identity operator r^0 for a given two-body
235 total spin S and a fixed pair of isospin projections is
236 $\mathcal{O}(r)[S, t_{za}, t_{zb}] = r^0[S, t_{za}, t_{zb}] \equiv \mathbf{1} P_S P_{t_{za}, t_{zb}}$, where the
237 identity is the same as in Eq. (13). Applying this opera-
238 tor to the A -nucleon space, the expectation value

$$\langle r^0[S, t_{za}, t_{zb}] \rangle = \sum_{\text{all } q\#} \sum_{i<j}^A ij \langle \alpha\beta; J | P_S P_{t_{za}, t_{zb}} | \gamma\delta; J \rangle_{ij}. \tag{20}$$

239 Summing over S in Eq. (20),

$$\begin{aligned}
\langle r^0[t_{za}, t_{zb}] \rangle &= \sum_{i<j}^A \sum_{\text{all } q\#} ij \langle \alpha\beta; J | \mathbf{1} | \gamma\delta; J \rangle_{ij} \delta_{t_{z\alpha}, t_{z\gamma}} \\
&\times \delta_{t_{z\beta}, t_{z\delta}} [\delta_{t_{z\alpha}, t_{za}} \delta_{t_{z\beta}, t_{zb}} + (1 - \delta_{t_{za}, t_{zb}}) \delta_{t_{z\alpha}, t_{zb}} \delta_{t_{z\beta}, t_{za}}] \\
&= \sum_{i<j}^A \sum_{t_{z\alpha}, t_{z\beta}} [\delta_{t_{z\alpha}, t_{za}} \delta_{t_{z\beta}, t_{zb}} + (1 - \delta_{t_{za}, t_{zb}}) \delta_{t_{z\alpha}, t_{zb}} \delta_{t_{z\beta}, t_{za}}],
\end{aligned} \tag{21}$$

240 which is an integer equal to the number of pairs with
241 a given pair of isospin projections (It is not an integer
242 before summing over S). It will become more clear when
243 we present the calculation results in Sec. IV A.

244 Considering all possible isospin projection pair configurations, 245 of-mass of all the nucleons are [30]

$$\begin{aligned}
\langle r^0 \rangle &= \sum_{t_{za} \leq t_{zb}} \langle r^0[t_{za}, t_{zb}] \rangle \\
&= \sum_{i < j} \sum_{t_{za} \leq t_{zb}} \sum_{t_{z\alpha}, t_{z\beta}} [\delta_{t_{z\alpha}, t_{za}} \delta_{t_{z\beta}, t_{zb}} + (1 - \delta_{t_{za}, t_{zb}}) \\
&\quad \times \delta_{t_{z\alpha}, t_{zb}} \delta_{t_{z\beta}, t_{za}}] \\
&= \sum_{i < j} 1 = \frac{A(A-1)}{2},
\end{aligned} \tag{22}$$

246 which is the total number of nucleon pairs when evaluated within states of an A -nucleon system. 247

248 E. Square-separation operator

249 The expectation value of the square-separation operator r^2 in the two-body space describes the relative 250 distance squared for a pair of nucleons. The square-separation operator for a fixed pair of isospin values 251 and a fixed two-body total spin S can be defined as 252 $\mathcal{O}(r)[S, t_{za}, t_{zb}] = r^2[S, t_{za}, t_{zb}] \equiv r^2 P_S P_{t_{za}, t_{zb}}$. Its expectation value in an A -body space 253

$$\langle r^2[S, t_{za}, t_{zb}] \rangle = \sum_{\text{all } q \neq i < j} \sum_{i < j} \langle ij | \alpha\beta; J | r^2 P_S P_{t_{za}, t_{zb}} | \gamma\delta; J \rangle_{ij}. \tag{23}$$

254 We recall the relative mean-square-radius operator for a system of A nucleons [30, 31] (also called the mean-square intrinsic coordinate operator in Ref. [29]) 255

$$r_{\text{rel}}^2 \equiv \frac{1}{A} \sum_i (\vec{r}_i - \vec{R}_{\text{cm}})^2 = \frac{1}{A^2} \sum_{i < j} (\vec{r}_i - \vec{r}_j)^2 = \frac{1}{A^2} r_A^2, \tag{24}$$

259 where the center-of-mass coordinates $\vec{R}_{\text{cm}} = (\sum_i^A \vec{r}_i)/A$. To calculate the point-proton/neutron rms radius, it is 260 convenient to first consider the corresponding relative mean-square-radius operator in each isospin projection 261 pair sector (pp , pn and nn) [32], $r_{\text{rel}, pp}^2 \equiv r_A^2[1/2, 1/2]/A^2$, 262 $r_{\text{rel}, pn}^2 \equiv r_A^2[1/2, -1/2]/A^2 = r_A^2[-1/2, 1/2]/A^2$ and 263 $r_{\text{rel}, nn}^2 \equiv r_A^2[-1/2, -1/2]/A^2$, where 264

$$\begin{aligned}
r_A^2[t_{za}, t_{zb}] &= \sum_{i < j} \langle ij | \alpha\beta; J | r^2 | \gamma\delta; J \rangle_{ij} \delta_{t_{z\alpha}, t_{z\gamma}} \delta_{t_{z\beta}, t_{z\delta}} \\
&\quad \times [\delta_{t_{z\alpha}, t_{za}} \delta_{t_{z\beta}, t_{zb}} + (1 - \delta_{t_{za}, t_{zb}}) \delta_{t_{z\alpha}, t_{zb}} \delta_{t_{z\beta}, t_{za}}]
\end{aligned} \tag{25}$$

265 is the square-separation operator projecting on a given isospin pair in an A -body space. The mean-square radius operators for protons and neutrons relative to the center-

$$r_p^2 \equiv \frac{1}{Z} \sum_i^A \delta_{t_{zi}, 1/2} (\vec{r}_i - \vec{R}_{\text{cm}})^2, \tag{26}$$

$$r_n^2 \equiv \frac{1}{N} \sum_i^A \delta_{t_{zi}, -1/2} (\vec{r}_i - \vec{R}_{\text{cm}})^2.$$

270 It can be easily shown that [32]

$$\begin{aligned}
r_p^2 &= (2A/Z - 1)r_{\text{rel}, pp}^2 + (A/Z - 1)r_{\text{rel}, pn}^2 - r_{\text{rel}, nn}^2, \\
r_n^2 &= -r_{\text{rel}, pp}^2 + (A/N - 1)r_{\text{rel}, pn}^2 + (2A/N - 1)r_{\text{rel}, nn}^2,
\end{aligned} \tag{27}$$

271 where A , Z and N are the nucleon, proton and neutron numbers, respectively. Then the point-proton (neutron) rms radius r_p (r_n) can be calculated by taking the 272 square root of the expectation value of r_p^2 (r_n^2). The point-nucleon matter rms radius r_m can be calculated 273 by taking the square root of the expectation value of r_m^2 (also denoted as r_m^2), or by utilizing the relation 274 $Ar_m^2 = Zr_p^2 + Nr_n^2$. 275

276 III. *AB INITIO* NCSM CALCULATION USING MFDn

277 In the *ab initio* NCSM, we consider a system of point-like non-relativistic nucleons that interact by realistic inter-nucleon interactions. The two-nucleon or 278 two-nucleon combining with three-nucleon interaction is taken from fitting two-nucleon phase shifts with high precision up to a certain energy and adjusting the remaining 279 parameters of the three-nucleon interaction to a selection of three-nucleon observables. Although we do not employ the three-nucleon interactions explicitly [33–35], we 280 plan to employ them in future studies that go beyond the scope of this work. 281

282 As the name NCSM implies, all the nucleons are considered active without an inert core that is assumed in 283 standard, valence space, shell model calculations. The Hamiltonian operator for an A -nucleons system is thus 284

$$H_A = \sum_{i < j}^A \frac{(\vec{p}_i - \vec{p}_j)^2}{2m_N A} + \sum_{i < j}^A V_{ij} + \sum_{i < j < k}^A V_{ijk} + \dots \tag{28}$$

285 where V_{ij} is the two-nucleon interaction, V_{ijk} is the three-nucleon interaction, and so on. 286

287 We solve the eigenvalue problem

$$H_A |\Phi_A\rangle = E |\Phi_A\rangle \tag{29}$$

288 in the harmonic-oscillator (HO) basis with energy spacing between shells $\hbar\Omega$ and many-body truncation N_{max} (the quanta of each shell is $2n + l$, where n and l are the 289 radial and orbital angular momentum quantum numbers, respectively; N_{max} defines the maximum total number of 290 quanta allowed in the many-body basis states for this

305 nucleus above the minimum required by the Pauli prin-
306 ciple).

307 The calculations are carried out using MFDn (Many-
308 Fermion Dynamics–nuclear), a configuration interaction
309 (CI) code for nuclear structure calculations [36, 37]. It is
310 a platform-independent Fortran 90 code using a hybrid
311 MPI/OpenMP programming model, and is being used on
312 current supercomputers, such as Cori and Perlmutter at
313 NERSC, for *ab initio* calculations of atomic nuclei using
314 realistic interactions.

315 We adopt the Daejeon16 two-nucleon (NN) interaction
316 [38] in our *ab initio* NCSM calculations. This interaction
317 is obtained by softening the chiral effective field theory
318 (χ EFT) generated Idaho next-to-next-to-next-to-leading
319 order (N3LO) NN interaction using the similarity renor-
320 malization group (SRG) method [39, 40]. A special fea-
321 ture of this interaction is that it is an NN interaction that
322 attempts to absorb the effects of interactions that might
323 otherwise be treated as three and higher many-body
324 forces, through phase-equivalent transformations (PETs)
325 [41]. The optimal set of PET parameters are obtained by
326 fitting the binding energies and spectra of selected light
327 nuclei up to ^{16}O . The Daejeon16 interaction provides a
328 good convergence rate in *ab initio* calculations for light
329 nuclei compared with other realistic interactions [42, 43].
330 Ground state energies and radii calculated using this in-
331 teraction are in reasonable agreement with the results of
332 experiments for p -shell nuclei [44]. Recently, the applica-
333 tions of Daejeon16 have been extended to medium and
334 heavy nuclei [45] using a mean-field with the inclusion of
335 a phenomenological 3-body contact interaction. In addition,
336 the Daejeon16 interaction has found many applica-
337 tions in scattering and resonances using the single-state
338 HO representation of scattering equations (SS-HORSE)
339 method [46–50].

340 The Daejeon16 interaction we use in this work has a
341 maximum total angular momentum cut-off $J_{\text{max}} = 6$. Be-
342 cause NN interactions are short-range and we are inter-
343 ested in only the ground states of these light nuclei, con-
344 tributions from larger values of J to the expectation value
345 of $\mathcal{O}(r)$ are anticipated to be vanishingly small. In ad-
346 dition, we superimpose the Coulomb interaction between
347 protons onto the Daejeon16 NN interaction since the con-
348 struction of Daejeon16 interaction is charge/isospin inde-
349 pendent.

350 After obtaining the matrix elements of operators
351 $O(r) = r^0$ and $O(r) = r^2$ in the HO basis (Appendix A),
352 we then take the additional step to transform these ma-
353 trix elements from the two-body relative frame to two-
354 body matrix elements in the single-particle basis by the
355 Moshinsky transformation sketched in Appendix B. The
356 resulting two-body matrix elements are then employed
357 to calculate expectation values using many-body NCSM
358 wavefunctions.

359 To determine suitable parameters of many-nucleon ba-
360 sis space cutoff N_{max} and HO energy spacing in the *ab*
361 *initio* NCSM calculation $\hbar\Omega$, we calculate r_p , r_n and r_m
362 in a grid of N_{max} from 6 to 18 with a step size of 2, and
363 $\hbar\Omega$ from 10 to 30 MeV with an increment of 2.5 MeV at
364 a time. Two additional points at the lower end of $\hbar\Omega$ (8
365 and 9 MeV) are also calculated, to show the rapid grow-
366 ing trend at lower $\hbar\Omega$ (except $N_{\text{max}} = 18$, for its relative
367 flatter trend around $\hbar\Omega = 10$ MeV at $N_{\text{max}} = 18$ com-
368 pared with lower N_{max} and the higher computational cost
369 associated with each point at $N_{\text{max}} = 18$; more points
370 will be calculated in future works when we perform an
371 extrapolation, and we are currently satisfied with those
372 points to give us an rough estimation of the uncertainty).
373 The results are shown in Fig. 1. Using these results as
374 a reference, we select $N_{\text{max}} = 16$ and $\hbar\Omega = 10$ MeV
375 for calculating the expectation values of the pair-identity
376 operator and the square-separation operator, which will
377 then be combined to give the mean square separation.
378 $\hbar\Omega = 10$ to 27.5 MeV is found to provide an approxi-
379 mate N_{max} independence for the point-nucleon rms radii
380 for ^4He , which can be seen in Fig. 2 through the al-
381 most invisible differences in the point-nucleon rms radii
382 (Δr) between $N_{\text{max}} = 16$ and $N_{\text{max}} = 18$. For ^6He ,
383 the current calculations do not show a good convergence
384 pattern. Meanwhile, Δr seems to decrease to 0 faster
385 at lower $\hbar\Omega$, inferred by Δr between $N_{\text{max}} = 14$ and
386 $N_{\text{max}} = 16$ (gray points). We choose $\hbar\Omega = 10$ to main-
387 tain an approximate convergence for ^4He while squeezing
388 the differences of the point-nucleon rms radii values be-
389 tween neighboring N_{max} for ^6He . $N_{\text{max}} = 16$ is chosen
390 because it is sufficient for our demonstration goal and
391 reasonable regarding the total computational resources
392 needed. By comparing the rms radii for $\hbar\Omega = 10$ MeV
393 from $N_{\text{max}} = 18$ with those from $N_{\text{max}} = 16$ (Fig. 2),
394 we estimate that the error of point-nucleon rms radii due
395 to basis truncation $N_{\text{max}} = 16$ with $\hbar\Omega = 10$ MeV are
396 $10^{-2} \sim 10^{-1}$ fm for ^6He and 10^{-3} fm for ^4He .

397 One interesting thing to note is that the $\hbar\Omega$ corre-
398 sponding to the minimum difference of point-nucleon rms
399 radius between $N_{\text{max}} = 18$ and $N_{\text{max}} = 16$ is not always
400 identical across r_p , r_n and r_m . For example, in ^4He , the
401 corresponding $\hbar\Omega = 15$ MeV for $r_{p/m}$ and 17.5 MeV for
402 r_n . We also note that these $\hbar\Omega$ are generally smaller than
403 the $\hbar\Omega$ for the minimum energy gap between $N_{\text{max}} = 18$
404 and $N_{\text{max}} = 16$. For instance, in ^4He , $\hbar\Omega = 17.5$ MeV
405 at the minimum energy gap, slightly greater than the $\hbar\Omega$
406 at the minimum $r_{p/m}$ gap. In ^6He , $\hbar\Omega = 12.5$ MeV at
407 the minimum energy gap is larger than the $\hbar\Omega$ at the
408 minimum $r_{p/n/m}$ gap (less than 10 MeV). With the ob-
409 servation that the minimum energy gap for ^4He and ^6He
410 moves towards a smaller $\hbar\Omega$ as basis size (N_{max}) increases
411 (Fig. 3), it seems that point-nucleon rms radii are more
412 sensitive to the changing of basis size compared with the
413 ground state energy.

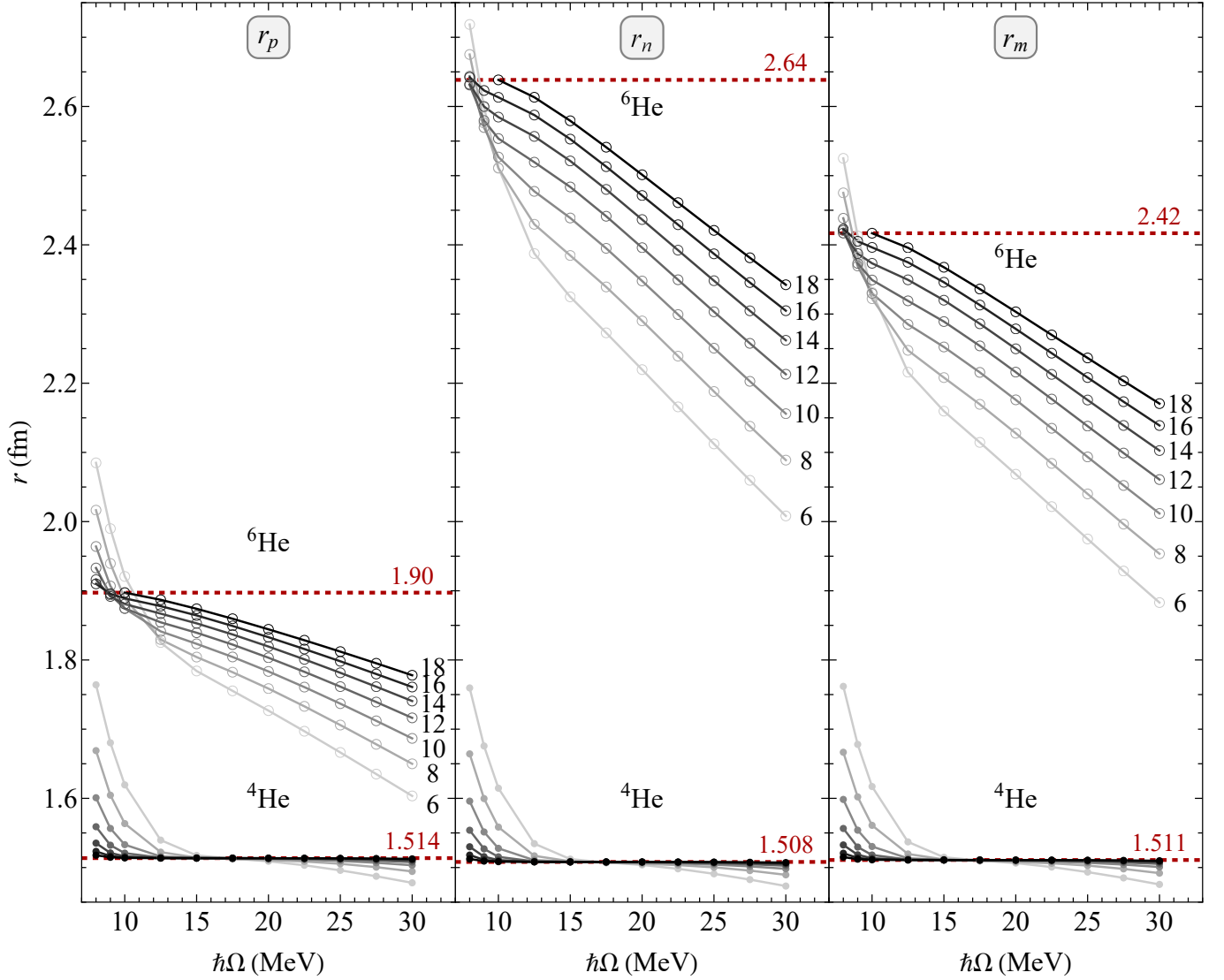


FIG. 1. r_p , r_n and r_m of ${}^4\text{He}$ and ${}^6\text{He}$ with Daejeon16 interaction plus Coulomb potential, calculated by MFDn for *ab initio* NCSM. Results for ${}^4\text{He}$ (${}^6\text{He}$) are represented by filled (open) circles, which are connected by a sequence of straight lines for the same N_{max} . The N_{max} values for ${}^6\text{He}$ are shown on the right of the sequences of lines, with increasing opacity as N_{max} increases. The horizontal dashed lines in each panel indicate the $r_{p/n/m}$ values of ${}^4\text{He}$ and ${}^6\text{He}$ for $N_{\text{max}} = 18$ with $\hbar\Omega$ corresponding to the minimum gap between the calculated points for $N_{\text{max}} = 18$ and $N_{\text{max}} = 16$ (in ${}^4\text{He}$, $\hbar\Omega = 15$ MeV for $r_{p/m}$ and $\hbar\Omega = 17.5$ MeV for r_n ; in ${}^6\text{He}$, $\hbar\Omega = 10$ MeV.).

IV. RESULTS AND ANALYSIS

A. The expectation value of pair-identity operator

The expectation value of a pair-identity operator $\langle r^0[S, t_{za}, t_{zb}] \rangle$ provides the probability of finding a pair of nucleons with fixed two-body total spin S and given isospin projections $\{t_{za}, t_{zb}\}$. The results of $\langle r^0[S, t_{za}, t_{zb}] \rangle$ for both values of S and for all the $\{t_{za}, t_{zb}\}$ combinations are presented in Table I.

Let us first perform a sanity check for the sum of $\langle r^0[S, t_{za}, t_{zb}] \rangle$ over all $\{S, t_{za}, t_{zb}\}$ combinations for ${}^4\text{He}$ and ${}^6\text{He}$ in the last row of Table I and confirm that

they are equal to the total number of nucleon pairs $A(A-1)/2$ for each nucleus as indicated by Eq. (22). We note that although the calculated $\langle r^0[S, t_{za}, t_{zb}] \rangle$ are not integers, a sum of $\langle r^0[S, t_{za}, t_{zb}] \rangle$ over two-body total spin S equals to an integer number of pairs with given $\{t_{za}, t_{zb}\}$ in ${}^4\text{He}$ and ${}^6\text{He}$, as suggested in Eq. (21). For example, both $\langle r^0[0, 1/2, 1/2] \rangle_{{}^4\text{He}} = 0.976772$ and $\langle r^0[1, 1/2, 1/2] \rangle_{{}^4\text{He}} = 0.023228$ are non-integers, while $\langle r^0[1/2, 1/2] \rangle_{{}^4\text{He}} = 0.976772 + 0.023228 = 1.000000$, recovering an integer number (within 5 significant digits).

We expect and find that *pp* and *nn* in the ground state of ${}^4\text{He}$ are dominantly spin-singlet, because this is the only $l = 0$ basis state (*s*-state) respecting the overall anti-

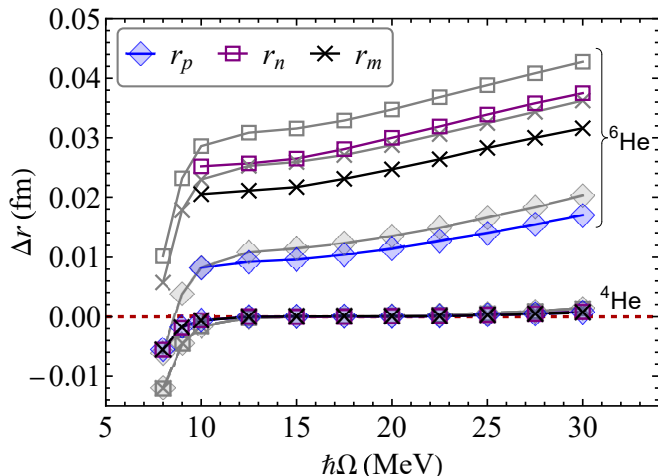


FIG. 2. Δr obtained by subtracting $r_{p/n/m}$ for $N_{\max} = 18$ ($N_{\max} = 16$) from those for $N_{\max} = 16$ ($N_{\max} = 14$), shown in color (gray) points. The absolute value $|\Delta r|$ serves as an indicator of the major source of the uncertainty of $r_{p/n/m}$ for ${}^4\text{He}$ and ${}^6\text{He}$ at $N_{\max} = 16$ in the *ab initio* NCSM calculation.

TABLE I. $\langle r^0[S, t_{za}, t_{zb}] \rangle$ for ${}^4\text{He}$ and ${}^6\text{He}$ with $N_{\max} = 16$ and $\hbar\Omega = 10$ MeV using the Daejeon16 interaction plus Coulomb potential, calculated by MFDn with an accuracy of 5 significant digits (denoted as “calc.”). To display these numbers in a uniform format, 6 decimal digits are shown (digits after the significant digits are grayed out). The naively expected value (denoted as “naive”) of each calculated result, based on occupying only the lowest available states in a HO basis, is listed for comparison as discussed in the text. The sum of each column is shown in the last line, which is equal to the number of pairs $A(A-1)/2$ for each nucleus.

		${}^4\text{He}$		${}^6\text{He}$	
	S	naive	calc.	naive	calc.
pp	0	1	0.976772	1	0.967578
pp	1	0	0.023228	0	0.032422
pn	0	1	0.979111	2	1.977430
pn	1	3	3.020890	6	6.022570
nn	0	1	0.976774	3	2.865420
nn	1	0	0.023226	3	3.134580
#pairs		6	6.000001	15	15.00000

438 symmetrization for exchanging of two isospin-symmetric
 439 fermions, i.e. $(-1)^{l+S+T} = -1$, where l , S and T are the
 440 two-body total orbital angular momentum in the two-
 441 body relative frame (See Appendix B), two-body total
 442 spin and two-body total isospin, respectively. One may
 443 also expect, as we indeed find, a small but non-zero por-
 444 tion of triplet (0.023228 for $\{pp, S = 1\}$ and 0.023226 for
 445 $\{nn, S = 1\}$) arising from partial wave contributions at
 446 higher values of l . The added Coulomb potential makes
 447 the isospin symmetry only approximate in our calcula-
 448 tions (note that we assume equal mass for the p and the

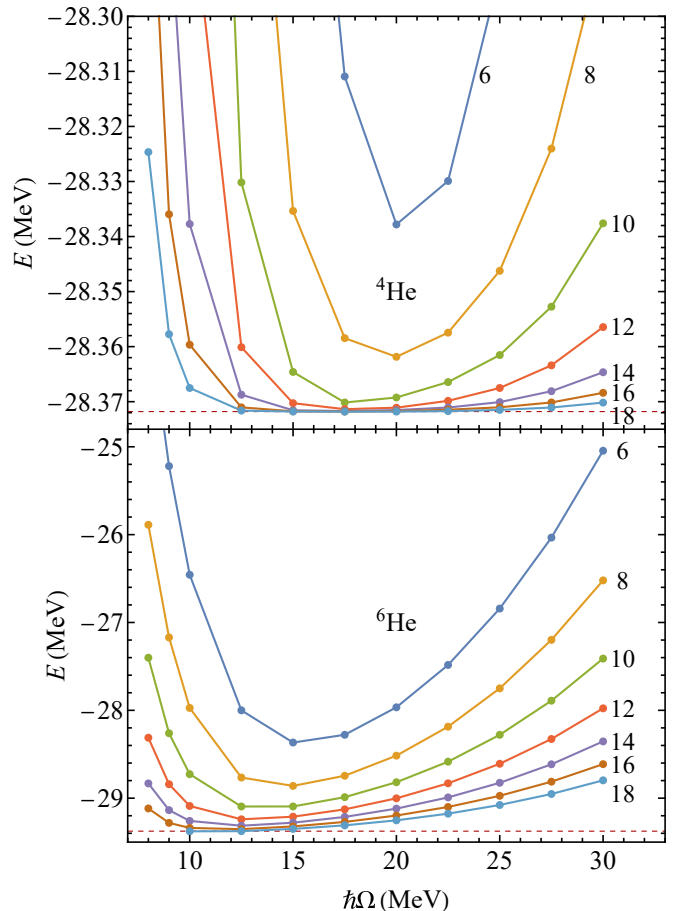


FIG. 3. The ground state energy with different N_{\max} and $\hbar\Omega$ for ${}^4\text{He}$ and ${}^6\text{He}$, using Daejeon16 interaction plus Coulomb potential, calculated by MFDn for *ab initio* NCSM. N_{\max} is labeled alongside the sequence of lines connecting the values calculated for the same N_{\max} . The horizontal dashed lines indicate the ground state energy of ${}^4\text{He}$ and ${}^6\text{He}$ for $N_{\max} = 18$ with $\hbar\Omega$ corresponding to the minimum gap between the calculated points for $N_{\max} = 18$ and $N_{\max} = 16$. In ${}^4\text{He}$, $\hbar\Omega = 17.5$ MeV; in ${}^6\text{He}$, $\hbar\Omega = 12.5$ MeV.

449 n which is taken as the average mass of these nucleons
 450 and Daejeon16 is charge-independent), which will con-
 451 tribute to the difference of expectation values between pp
 452 and nn pairs for ${}^4\text{He}$. However, this deviation should be
 453 small and consistent with the fact that isospin is known
 454 to be a very good symmetry for light nuclei, as revealed
 455 in the approximately balanced pp and nn results for ${}^4\text{He}$
 456 in Table I.

457 For the spin-independent parts of the NN interactions,
 458 singlet and triplet two-body spin states have the same
 459 energy in the same HO wave function of relative motion
 460 (labeled by n and l for two-body central potentials)—
 461 there is no preference among the allowed two-body spin
 462 configurations $\uparrow\uparrow$ (triplet), $\downarrow\downarrow$ (triplet), $\uparrow\downarrow + \downarrow\uparrow$ (triplet)
 463 and $\uparrow\downarrow - \downarrow\uparrow$ (singlet). As a result, the ratio of the prob-
 464 ability of triplet to singlet two-body spin states for the
 465 ground state of ${}^4\text{He}$ pn pairs is approximately 3:1. Upon

considering the spin-dependent part of the NN potential, e.g. $S_p S_n$ coupling in the s -state, which can be usefully written as $V_{\text{spin}} = \hbar^{-2} V_1(r) \vec{S}_p \cdot \vec{S}_n$ [51], the probability of finding an pn pair in one of the triplet states can be slightly larger than in the singlet state if $V_1(r)$ is effectively attractive (thus negative), as in deuterium. This assessment takes into account that $\langle \vec{S}_p \cdot \vec{S}_n \rangle = +\hbar^2/4$ for triplet states and $-\hbar^2/4$ for singlet states. These expectations are met, as can be seen in the calculated pn results of ${}^4\text{He}$ in Table I.

We then inspect $\langle r^0[S, t_{za}, t_{zb}] \rangle$ of ${}^6\text{He}$ in Table I. To pave the way for later discussions, we digress a bit to highlight the difference between ${}^4\text{He}$ and ${}^6\text{He}$ when their constituent nucleons occupy the lowest possible single-particle states of a HO basis. Unlike ${}^4\text{He}$, at the ground state of ${}^6\text{He}$, there are two additional neutrons that are unable to occupy the lowest single-particle state due to the Pauli exclusion principle. This can be immediately seen from the ground state proton and neutron occupation probabilities (Fig. 4). For ${}^4\text{He}$, the two lowest s -states ($0s_{1/2}$ and $1s_{1/2}$) contribute about 90% of the total occupation number, which is 2 for either protons or neutrons. For ${}^6\text{He}$, these two states still contribute about $1.74/2=87\%$ of the proton number, but only gather about $1.83/4=46\%$ of the neutron number. On the other hand, the occupancy of neutrons at $0p_{1/2}$ ($0p_{3/2}$) is 0.22 (1.70), which contributes 5% (43%) of the neutron number. This suggests that, in ${}^6\text{He}$, two neutrons largely remain in the lowest two single-particle s -states (mainly $0s_{1/2}$, with 1.73 occupancy)—regarded as the “ α core” neutrons, and the other two neutrons are mainly in the $0p_{3/2}$ state—regarded as the valence neutrons.

Following the analyses above, it turns out that the calculated $\langle r^0[S, t_{za}, t_{zb}] \rangle$ of ${}^6\text{He}$ in Table I are consistent with the naive expectations described below, with a maximum deviation of 0.14, which is small on these scales. pp should largely stay at the singlet state, inferred by the moderate change of proton occupancy from ${}^4\text{He}$ to ${}^6\text{He}$ (Fig. 4). The two “ α core” neutrons of ${}^6\text{He}$ shall correlate similarly as the ${}^4\text{He}$ neutrons do with the protons. In other words, it is thrice as likely to find a triplet state than to find a singlet state in the pn pairs within the “ α core”. Among the eight pn pairs of ${}^6\text{He}$, the ratio of triplet states to singlet states in the other four pn pairs might be the same as the “ α core” pn pairs. The reason is as follows. Since for ${}^6\text{He}$ neutrons, $0s_{1/2}$ and $0p_{3/2}$ states are approximately equal in contribution, while the rest of states are highly suppressed, we can consider the “ α core” neutrons and the valence neutrons as two groups only differing by unperturbed orbitals occupied. Therefore, when neutrons in each group form two-body total spin with the protons, ideally, there should be again no preference among the four two-body total spin states, $\uparrow\uparrow$ (triplet), $\downarrow\downarrow$ (triplet), $\uparrow\downarrow + \downarrow\uparrow$ (triplet) and $\uparrow\downarrow - \downarrow\uparrow$ (singlet). In addition, the two protons can be regarded as the third group with the same nucleon occupancy. The two-body total spin states in nn pairs formed by inter-group neutrons (one n comes from the “ α core” and the

other n comes from the valence shell) shall mimic the ones in pn pairs. Multiplying the total number pairs by the probability of taking each two-body total spin state, we expect three nn pairs in triplet states and one nn pair in singlet states, for nn pairs formed by inter-group neutrons. To a lesser extent, we shall also expect to have another two nn pairs in singlet states, one formed by the two “ α core” neutrons and the other formed by the two valence neutrons, assuming the correlations of neutrons within each shell are more important than correlations of neutrons across different shells. This assumption shall be mostly true, because the difference between the expected and calculated $\langle r^0[S, t_{za}, t_{zb}] \rangle$ for ${}^6\text{He}$ nn pairs in Table I is only 0.14, which is small on these scales.

It is interesting to note that when we exclude the ${}^6\text{He}$ nn pairs in our consideration, the largest deviation between the calculated results and their naively expected integer values is only 0.033 for ${}^6\text{He}$ and 0.024 for ${}^4\text{He}$. This is consistent with our speculation that the two valence neutrons have an insignificant influence on the “ α core” two-body total spin configurations. Fig. 5 is a possible arrangement of the spin and orbital angular momentum of the two valence neutrons of ${}^6\text{He}$ speculated from Fig. 4(b), for the ground state dominant configuration satisfying $\vec{S} = \vec{s}_1 + \vec{s}_2 = 0$, where \vec{s}_1 and \vec{s}_2 are the spin of the two valence neutrons. It should be noted that the real picture for the orbital rotation is more complicated, because at least the center-of-mass motion should be supplemented to this simplified picture. As a consequence, for the ground state with $l = 0$, the orbital angular momentum of the two valence neutrons (\vec{l}_1 and \vec{l}_2) are not necessarily antiparallel, i.e., \vec{l}_1 and \vec{l}_2 contain information of the residual center-of-mass motion.

We now address the role of N_{max} truncation. The maximum difference of $\langle r^0[S, t_{za}, t_{zb}] \rangle$ between $N_{\text{max}} = 16$ and $N_{\text{max}} = 14$ is 1×10^{-4} for ${}^6\text{He}$ pp/pn pairs and 5×10^{-4} for ${}^6\text{He}$ nn pairs. Keeping in mind that the MFDn calculation preserves 5 significant digits, it is meaningful that the dependence on basis truncation still resides in the 4th decimal digit of the results. On the other hand, for ${}^4\text{He}$, the maximum difference of $\langle r^0[S, t_{za}, t_{zb}] \rangle$ between $N_{\text{max}} = 16$ and $N_{\text{max}} = 14$ is 4×10^{-5} , so the uncertainty due to truncation that we quote only appears in the 5th decimal digit.

To investigate which two-body states dominate in $\langle r^0 \rangle$, we examine the major two-body states (labeled by spectroscopic notation $n^{2S+1}l_J$, where $|l - S| \leq J \leq |l + S|$) of $\langle r^0 \rangle$ for the three isospin-projected pair configurations, shown in Fig. 6. For ${}^4\text{He}$ ground state, all the major components come from s -states, as naively expected from the shell model. ${}^4\text{He}$ pp is mostly (81%) at the lowest singlet state, with a small portion (12%) at the $n = 1$ singlet s -state. ${}^6\text{He}$ pp is almost identical to ${}^4\text{He}$. ${}^4\text{He}$ pn triplet states are dominated by the lowest two s -states (96%), while ${}^4\text{He}$ pn singlet is dominated by the lowest s -state (81%). For ${}^6\text{He}$ pn pairs, we see the rising of p/d -states in both singlet and triplet configurations. The three major p -states contribute 22% and the 0^3d_3 state contributes

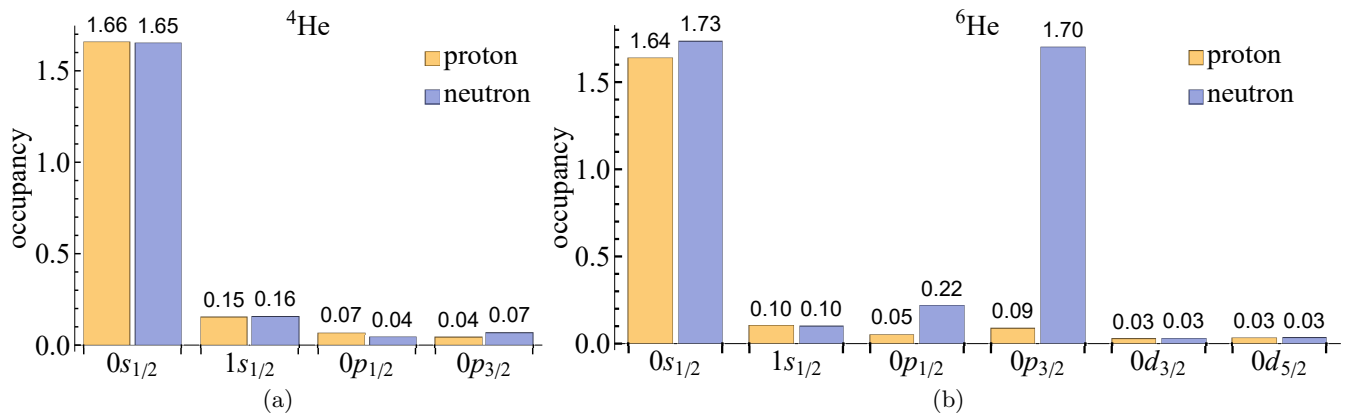


FIG. 4. Occupancy of protons or neutrons on single-particle states for the ground state ${}^4\text{He}$ (a) and ${}^6\text{He}$ (b), with $N_{\text{max}} = 16$ and $\hbar\Omega = 10$ MeV. The single-particle states that are major contributors are shown, which collectively contribute more than 90% of the proton number or neutron number of each nucleus.

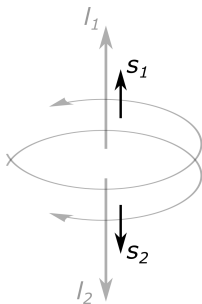


FIG. 5. The sketch of a possible arrangement for the the spin and orbital angular momentum of the two valence neutrons of ${}^6\text{He}$ in the ground state dominant configuration.

1% of $\langle r^0 \rangle$. For nn , we again see the rising of higher states (45% p -states and 2% 0^1d_2) in ${}^6\text{He}$. We note that, for nn , due to the $(-1)^{l+S+T} = -1$ antisymmetry constraint, all allowed p -states are triplets and all allowed s/d -states are singlets. It follows that, ${}^6\text{He}$ nn triplets are dominantly at p -states and ${}^6\text{He}$ nn singlets are dominantly at s -states.

To sum up, we conclude that the two ${}^6\text{He}$ valence neutrons dominantly form a singlet spin configuration and mostly in s -states, from the consideration of preserving ${}^4\text{He}$ two-body total spin configuration inside ${}^6\text{He}$ (suggested by the fact that the proton/neutron occupation probabilities at $0s_{1/2}$ single particle state in Fig. 4 and pp two-body spin states in Fig. 6(a) remain almost unchanged from ${}^4\text{He}$ to ${}^6\text{He}$), and from the fairly good consistency between the *ab initio* NCSM calculated $\langle r^0 \rangle$ and the naively expected values (Table I). This provides an indicator of halo structure in ${}^6\text{He}$ through the following reasoning. The nn singlet s -states have symmetrical spatial wave functions Ψ_{nlm} which have non-zero probability close to the center-of-mass of the pair due to the absence of a centrifugal term in the relative Schrödinger equation, resulting in a stronger correlation between the two nucleons compared with triplet states. This seems to support

a “di-neutron” halo at some distance from the center-of-mass of the nucleus. The “cigar”-like configuration is another possibility seen in many calculations but appears not to be the dominant configuration [1, 52, 53].

It can be seen from the above analyses that the *ab initio* NCSM calculated $\langle r^0 \rangle$ is useful for speculating the structure of the ground state ${}^6\text{He}$. These analyses are quantitatively limited by the symmetry assumptions involved. We assume the ${}^4\text{He}$ two-body total spin configuration is preserved inside ${}^6\text{He}$. We further assume the equal probabilities of taking the four possible two-body spin configurations ($\uparrow\uparrow$, $\downarrow\downarrow$, $\uparrow\downarrow + \downarrow\uparrow$, $\uparrow\downarrow - \downarrow\uparrow$) for pn or nn pairs that are “indistinguishable”, where “indistinguishable” between two nucleon pairs means that each p or n in one nucleon pair comes from the same group as a p or n in the other nucleon pair, and vice versa (one-to-one correspondence). As mentioned above, there are three groups of nucleons in ${}^6\text{He}$, “ α core” neutrons, valence neutrons and protons. To mitigate the impact of these assumptions, we quantitatively investigate the single-particle state occupation probabilities and the major two-body spectroscopic components of $\langle r^0 \rangle$ in this section. Another route brings in the results of the other operators for relaxing these symmetry constraints as demonstrated in the coming section Sec. IV B.

B. The expectation value of square-separation operator

The expectation values of the square-separation operator for different two-body total spin and isospin projections $\langle r^2[S, t_{za}, t_{zb}] \rangle$ are presented in Table II. To normalize $\langle r^2[S, t_{za}, t_{zb}] \rangle$ to its average value for a single pair of nucleons, we define the mean square separation between two nucleons of given $\{S, t_{za}, t_{zb}\}$ as

$$\overline{\langle r^2[S, t_{za}, t_{zb}] \rangle} \equiv \frac{\langle r^2[S, t_{za}, t_{zb}] \rangle}{\langle r^0[S, t_{za}, t_{zb}] \rangle}, \quad (30)$$

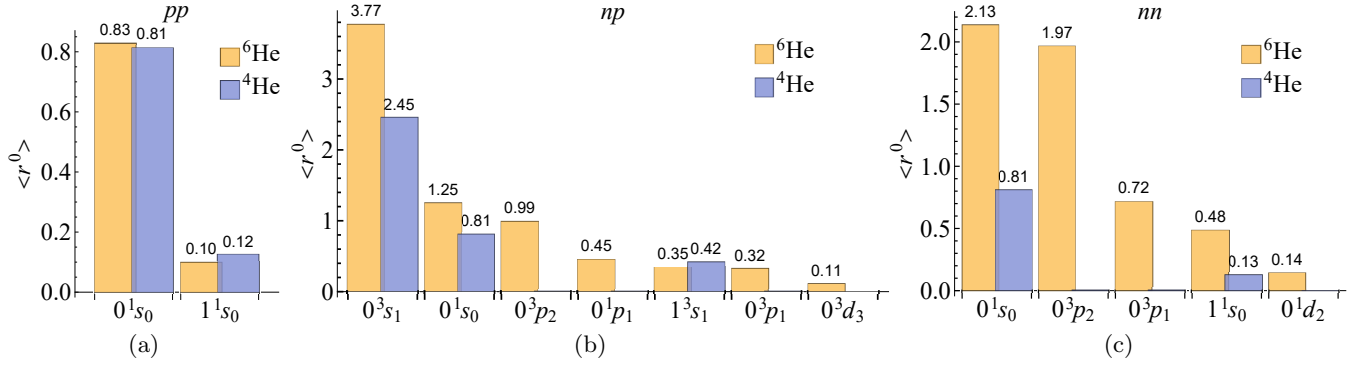


FIG. 6. Major $\langle r^0 \rangle$ two-body contributions of the ground state ${}^4\text{He}$ and ${}^6\text{He}$ with $N_{\text{max}} = 16$ and $\hbar\Omega = 10$ MeV, for pp (a), pn (b) and nn (c) pair configurations. The bins are arranged in decreasing order for ${}^6\text{He}$, with the corresponding ${}^4\text{He}$ bins shown alongside for comparison. The above shown states in total contribute more than 90% of $\langle r^0 \rangle$ in each isospin-projected pair configuration.

639 and the rms separation between two nucleons of given
640 $\{S, t_{za}, t_{zb}\}$

$$\overline{\langle r^2[S, t_{za}, t_{zb}] \rangle}^{1/2} \equiv \sqrt{\frac{\langle r^2[S, t_{za}, t_{zb}] \rangle}{\langle r^0[S, t_{za}, t_{zb}] \rangle}}. \quad (31)$$

641 These derived quantities are shown in the last two
642 columns for each nucleus in Table II.

TABLE II. $\langle r^2[S, t_{za}, t_{zb}] \rangle$ [fm²] for ${}^4\text{He}$ and ${}^6\text{He}$ with $N_{\text{max}} = 16$ and $\hbar\Omega = 10$ MeV using the Daejeon16 interaction plus Coulomb potential, calculated by MFDn with an accuracy of 5 significant digits (digits after the significant digits are grayed out). We also present in the second (third) column of each nucleus the mean square separation $\overline{\langle r^2[S, t_{za}, t_{zb}] \rangle}$ [fm²] (the rms separation $\overline{\langle r^2[S, t_{za}, t_{zb}] \rangle}^{1/2}$ [fm]). The last line shows the sum of $\langle r^2[S, t_{za}, t_{zb}] \rangle$ for each nucleus.

	${}^4\text{He}$			${}^6\text{He}$			
	S	$\langle r^2 \rangle$	$\overline{\langle r^2 \rangle}^{1/2}$	$\langle r^2 \rangle$	$\overline{\langle r^2 \rangle}$	$\overline{\langle r^2 \rangle}^{1/2}$	
pp	0	5.95862	6.10032	2.46988	6.63201	6.85424	2.61806
pp	1	0.22754	9.79581	3.12983	0.36145	11.1484	3.33892
pn	0	5.94563	6.07248	2.46424	24.5046	12.3921	3.52024
pn	1	18.3172	6.06352	2.46242	73.2384	12.1607	3.48721
nn	0	5.89396	6.03411	2.45644	38.7177	13.5121	3.67588
nn	1	0.22648	9.75110	3.12268	63.2643	20.1827	4.49252
sum		36.5695	-	-	206.718	-	-

643 These results can be interpreted with the following con-
644 siderations. Using again the overall antisymmetrization
645 property of fermion pairs as mentioned in Sec. IV A, the
646 rms separation for singlet is expected to be smaller than
647 triplet for the pp and nn pairs in their lowest partial
648 waves. This turns out to be true for both ${}^4\text{He}$ (2.5 fm
649 versus 3.1 fm) and ${}^6\text{He}$ (2.6 fm versus 3.3 fm for pp ; 3.7 fm
650 versus 4.5 fm for nn) seen in Table II. For pn pairs, since
651 the total two-body isospin T can be either 0 or 1, the spa-
652 tial part of the wave function for given S can be either

653 symmetric or antisymmetric. Thus, the rms separation
654 for singlet pn pairs and triplet pn pairs are similar (2.46
655 fm for both in ${}^4\text{He}$; 3.52 fm and 3.49 fm, in ${}^6\text{He}$).

656 Comparing ${}^6\text{He}$ with ${}^4\text{He}$, we see that the rms sep-
657 aration for pp singlet configuration, which is the dom-
658 inant two-body spin configuration of pp , is expanded
659 by 6% from ${}^4\text{He}$ to ${}^6\text{He}$. Interestingly, the remaining
660 $\sim 3\%$ (Table I) portion pp triplet states also experiences
661 a similar expansion in rms separation from ${}^4\text{He}$ to ${}^6\text{He}$,
662 even though they are negligible. On the other hand,
663 the rms separation for nn and pn pairs are expanded
664 by 40% \sim 50% from ${}^4\text{He}$ to ${}^6\text{He}$.

665 Summing over S in both denominator and numerator
666 of Eq. (30), we define the mean square separation for
667 nucleon pairs of given $\{t_{za}, t_{zb}\}$ as

$$\overline{\langle r^2[t_{za}, t_{zb}] \rangle} \equiv \frac{\sum_S \langle r^2[S, t_{za}, t_{zb}] \rangle}{\sum_S \langle r^0[S, t_{za}, t_{zb}] \rangle} = \frac{\langle r^2[t_{za}, t_{zb}] \rangle}{\langle r^0[t_{za}, t_{zb}] \rangle}. \quad (32)$$

668 ${}^4\text{He}$ and ${}^6\text{He}$ has only one pp , $\langle r^0[1/2, 1/2] \rangle_{{}^4\text{He}, {}^6\text{He}} =$
669 1. Similarly, it is straightforward to note that
670 $\langle r^0[-1/2, 1/2] \rangle_{{}^4\text{He}} = 4$, $\langle r^0[-1/2, 1/2] \rangle_{{}^6\text{He}} = 8$,
671 $\langle r^0[-1/2, -1/2] \rangle_{{}^4\text{He}} = 1$ and $\langle r^0[-1/2, -1/2] \rangle_{{}^6\text{He}} = 6$.
672 The rms separation of given $\{t_{za}, t_{zb}\}$ can be defined as
673 the square root of the above quantity. The calculated
674 mean square separations along with the rms separations
675 are shown in Table III, consistent with the corresponding
676 results computed using NNLO_{opt} nucleon-nucleon inter-
677 action [54] with $N_{\text{max}} = 14$ in Ref. [55] (${}^4\text{He}$ $\overline{\langle r^2 \rangle}_{pp}^{1/2} \approx$
678 2.40 fm; ${}^6\text{He}$ $\overline{\langle r^2 \rangle}_{pp}^{1/2} \approx 2.62$ fm, $\overline{\langle r^2 \rangle}_{pn}^{1/2} \approx 3.3$ fm and
679 $\overline{\langle r^2 \rangle}_{nn}^{1/2} \approx 3.9$ fm).

680 To describe a nucleus by nucleon-nucleon separation
681 without specifying nucleon species, we define the mean
682 square separation between two nucleons in a nucleus

$$\overline{\langle r^2 \rangle} \equiv \frac{\sum_{S, t_{za} \leq t_{zb}} \langle r^2[S, t_{za}, t_{zb}] \rangle}{\sum_{S, t_{za} \leq t_{zb}} \langle r^0[S, t_{za}, t_{zb}] \rangle} = \frac{\langle r^2 \rangle}{A(A-1)/2}, \quad (33)$$

TABLE III. $\langle r^2[t_{za}, t_{zb}] \rangle$ [fm²] computed from Table II, together with the mean square separation $\overline{\langle r^2[t_{za}, t_{zb}] \rangle}$ [fm²] and the rms separation $\overline{\langle r^2[t_{za}, t_{zb}] \rangle}^{1/2}$ [fm]. Digits after the 5 significant digits are grayed out.

	⁴ He			⁶ He		
	$\langle r^2 \rangle$	$\overline{\langle r^2 \rangle}$	$\overline{\langle r^2 \rangle}^{1/2}$	$\langle r^2 \rangle$	$\overline{\langle r^2 \rangle}$	$\overline{\langle r^2 \rangle}^{1/2}$
<i>pp</i>	6.18616	6.18616	2.48720	6.99346	6.99346	2.64452
<i>pn</i>	24.2629	6.06572	2.46287	97.7429	12.2179	3.49541
<i>nn</i>	6.12044	6.12044	2.47395	101.982	16.9970	4.12274

where $A(A-1)/2 = 6$ for ⁴He and $A(A-1)/2 = 15$ for ⁶He. Then the rms nucleon-nucleon separation within a nucleus is the square root of $\langle r^2 \rangle$. From Table II and Eq. (33), $\overline{\langle r^2 \rangle}_{4\text{He}} = 6.0949$ fm² and $\overline{\langle r^2 \rangle}_{6\text{He}} = 13.781$ fm², which yield $\overline{\langle r^2 \rangle}_{4\text{He}}^{1/2} = 2.4688$ fm and $\overline{\langle r^2 \rangle}_{6\text{He}}^{1/2} = 3.7123$ fm, meaning that the nucleon-nucleon separations of ⁶He, on average, are 50% larger than those of ⁴He.

One way to estimate the “halo” effect of ⁶He is to compare the neutron radius of ⁶He with ⁴He. One can make use of the calculated binding energy of ⁴He and ⁶He ($N_{\text{max}} = 16$, $\hbar\omega = 10$ MeV), which are -28.3597 MeV and -29.3387 MeV, respectively. Subtracting these two values gives two-neutron separation energy for ⁶He $\Delta E_s = 0.979$ MeV. From the characteristic wave number $k_{\text{ch}} = \sqrt{m_N \Delta E_s / \hbar^2} \sim 0.15$ fm⁻¹, the corresponding neutron radius is ~ 6.5 fm. Similarly, for ⁴He, $k_{\text{ch}} \sim 0.7$ fm⁻¹ can be obtained by additional *ab initio* NCSM calculations of ground state binding energy, e.g., -7.75 MeV for ³He (-8.44 MeV for ³H) with $N_{\text{max}} = 22$ and $\hbar\omega = 10(12.5)$ MeV (the ground state energy is nearly convergent at these N_{max} and $\hbar\omega$ values). Thus, the neutron and proton radius of ⁴He is about 1.4 fm. The discrepancy between the estimated neutron radius of ⁶He and ⁴He could signal the formation of a “halo” in ⁶He. However, the characteristic wave number is based on *s*-states. As shown in Fig. 6, *p/d*-states also play an important role in *nn* and *pn* pairs of ⁶He.

To make a more quantitative estimation of the “halo” effect of ⁶He, we compute and present in Table IV r_p , r_n and r_m for ⁴He and ⁶He, by combining the calculated $\langle r^2[t_{za}, t_{zb}] \rangle$ with Eq. (27), with $N_{\text{max}} = 16$ and $\hbar\Omega = 10$. r_p^* , r_n^* and r_m^* are the ones obtained with $N_{\text{max}} = 18$ and $\hbar\Omega$ corresponding to the minimum gap Δr between $N_{\text{max}} = 18$ and $N_{\text{max}} = 16$ (indicated in Fig. 1). Comparing $r_{p/n/m}$ and $r_{p/n/m}^*$ gives an estimation of the magnitude of the basis cut-off uncertainties. For ⁴He, the differences appear in the third decimal digit. For ⁶He, the differences show up in the second decimal digit.

The experimental point-nucleon rms radii are indicated in the last column of each nucleus in Table IV. The point-proton rms radius is calculated using $r_p^2 = r_c^2 - R_p^2 - 3/(4M_p^2) - (N/Z)R_n^2 - r_{so}^2$, where the nucleus

rms charge radius r_c can be measured from laser spectroscopy or scattering experiments, the Darwin-Foldy term $3/(4M_p^2) = 0.033$ fm² [56] and the neutron mean square charge radius $R_n^2 = -0.1161(22)$ [56]. The relativistic correction due to spin-orbit interaction $r_{so}^2 = 0$ for ⁴He and -0.08 fm² for ⁶He [57]. Considering the discrepancy between two groups of experimental proton charge radius after an experiment using muonic hydrogen atoms [58] (see Refs. [59, 60] for recent reviews), we present results calculated by two values of proton mean square charge radius, $R_p^2 = 0.7658(93)$ (CODATA 2016 [61]) and $R_p^2 = 0.7071(6)$ (PDG 2020 [56]), separated by a slash. The experimental range of r_m in Table IV is obtained from interaction cross sections of elastic scattering [62]. The experimental r_n is computed from the relation $Ar_m^2 = Zr_p^2 + Nr_n^2$. The point-nucleon rms radii are relatively well-converged for ⁴He but the desired fully convergent point-nucleon rms radii for ⁶He have not been achieved with this limited basis size. The calculation results are in reasonable agreement with the experimental values within the uncertainty ranges. The calculated ⁴He r_p is slightly larger than the experimental values by $0.02 \sim 0.06$ fm, with a moderate decreasing trend as basis size increases. The calculated ⁶He r_p is slightly smaller (by $0.01 \sim 0.07$ fm) than the experimental values while increasing as the basis size increases.

From Table IV, the calculated point-proton and point-neutron rms radii for ⁴He are nearly identical, around $r_0 = 1.51$ fm. And from Table III, ⁴He *pp*, *pn* and *nn* rms separations are also very similar, about $a = 2.47$ fm. The ratio $a/r_0 = 1.636$ is approximately the same as the side length to the center-to-vertex distance ratio of a tetrahedron $2\sqrt{6}/3 = 1.633$. This suggests a route by which we can relate our quantum many-body results to a classical picture that depicts ⁴He as a tetrahedron with protons and neutrons at the tetrahedron’s vertices.

In Table III, the *pp* rms separation of ⁶He increases by 6.3%, while the *pn* (*nn*) rms separation of ⁶He increases by 41.9% (66.6%), compared with those of ⁴He. It turns out that the main feature of these changes can be captured by a binary model. We introduce x (y) as the ratio between the rms separation of *pn* or *nn* consisting only of the “ α core” nucleons (contains at least one nucleon outside the “ α core”) in ⁶He and the rms separation of *pn* or *nn* in ⁴He, i.e.,

$$\frac{r_{pn/nn,i}^{(6\text{He})}}{r_{pn/nn}^{(4\text{He})}} = \begin{cases} x, & \text{both nucleons within the “}\alpha\text{ core”} \\ y, & \text{otherwise} \end{cases} \quad (34)$$

Matching the percentage increases,

$$\frac{r_{pn}^{(6\text{He})} - r_{pn}^{(4\text{He})}}{r_{pn}^{(4\text{He})}} = \sqrt{\frac{4x^2 + 4y^2}{8}} - 1 = 41.9\%, \quad (35)$$

and

$$\frac{r_{nn}^{(6\text{He})} - r_{nn}^{(4\text{He})}}{r_{nn}^{(4\text{He})}} = \sqrt{\frac{x^2 + 5y^2}{6}} - 1 = 66.6\%. \quad (36)$$

TABLE IV. The expectation value of $r_{p/n/m}^2$ [fm²] and $r_{p/n/m}$ [fm] for ⁴He and ⁶He, calculated by *ab initio* NCSM with $\hbar\Omega = 10$ MeV and $N_{\max} = 16$ using Daejeon16 plus Coulomb interaction. Digits after the 5 significant digits are grayed out. $r_{p/n/m}^*$ [fm] is the rms radius for $N_{\max} = 18$, with $\hbar\Omega$ corresponding to the minimum gap Δr between $N_{\max} = 18$ and $N_{\max} = 16$ (Fig. 1), served as a reference for the uncertainty owing to the N_{\max} truncation. The experimental values are shown in the last column of each nucleus, where r_p and r_m are separately measurable, and the experimental r_n is obtained using $Ar_m^2 = Zr_p^2 + Nr_n^2$.

	⁴ He				⁶ He			
x	r_x^2	r_x	r_x^*	$r_x(\text{exp.})$	r_x^2	r_x	r_x^*	$r_x(\text{exp.})$
p	2.29381	1.51453	1.5136	1.464(6)/1.484(5) [63]	3.56864	1.88908	1.8973	1.938(23)/1.953(22) [64]
n	2.27738	1.50910	1.5081	1.43–1.84	6.82895	2.61323	2.6384	2.35–3.08
m	2.28559	1.51182	1.5109	1.46–1.66 [62]	5.74218	2.39628	2.4168	2.23–2.75 [62]

Solving these two equations yields $x = 0.93$ and $y = 1.78$. This suggests that the pn/nn rms separation for the “ α core” stays nearly the same as for ⁴He, while the rms separation of pn/nn not belonging to the “ α core” is found to increase by almost 80%, indicating the formation of a halo.

It should be noted that the simple binary model treats the “ α core” as approximately a point mass when viewed by each of the two valence neutrons, ignoring the fact that the size of the “ α core” is comparable to the distance between the valence neutrons and the core. In fact, similar pictures are often adopted in current *ab initio* calculations where clustering information is input as a piece of prior knowledge.

Finally, we observe that the point-proton rms radius increases by 25% from ⁴He ($r_p = 1.515$ fm) to ⁶He ($r_p = 1.889$ fm) (Table IV). This increase may be understood as the consequence of a halo structure, arising from the motion of the charged “ α core” around the common center-of-mass as well as possible contributions from swelling of the “ α core” [62].

V. CONCLUSION AND ADDITIONAL DISCUSSIONS

We show that the formation of the halo structure of ⁶He can be examined from the coordinate-space two-body correlation operators. More specifically, we analyze the *ab initio* NCSM calculation results of the pair-identity operator (r^0) and the square-separation operator (r^2) for different nucleon pairs with fixed two-body total spin and two-body total angular momentum. We illustrate the dominant two-body spin configurations of ⁴He and ⁶He by analyzing the results of r^0 . We demonstrate that the inclusion of r^2 provides a more subtle picture of ⁶He, by utilizing the calculated point-nucleon rms radius and a binary model constructed using the calculated rms separations between nucleons.

We believe that the spatial correlation operators can refine our understanding of halo nuclei, beyond the general application of using them to calculate the point-nucleon rms radius r_p , r_n and r_m . This paper demonstrates the usefulness of r^0 and r^2 in analyzing the nu-

clear structure. We are also interested in exploring other spatial correlation operators, such as r^4 and r^6 , to see what additional information is available. In addition, we speculate there may be a systematic way to combine those spatial correlation results to provide a richer physical picture of the structure of light nuclei.

There is a need to develop robust extrapolation techniques for spatial correlation operators that are long-range and difficult to converge with increasing the basis size (N_{\max}). Even though both ⁴He and ⁶He ground state energy seems to saturate around the $\hbar\Omega$ corresponding to the variational minimum (Fig. 3), their point-nucleon rms radii present a more complicated pattern (Fig. 1). Ref. [65] proposed a two-dimensional twisted tape extrapolation using point-nucleon radii results from *ab initio* NCSM with Daejeon16 interaction plus Coulomb interaction for ⁶He (the largest basis for ⁶He adopted in this paper is the one with $N_{\max} = 14$). The finite N_{\max} point-nucleon rms radii for ⁴He in this paper are identical to ours, but the ones for ⁶He in this paper are slightly (~ 0.01 MeV) smaller than ours. The extrapolated point-nucleon rms radii in Ref. [65] for ⁶He are $r_p = 1.871(16)$ fm, $r_n = 2.663(3)$ fm and $r_m = 2.430(6)$ fm. This r_p is slightly smaller than our r_p for $N_{\max} = 16$ and $N_{\max} = 18$ (Table IV), which might partially result from their slightly smaller r_p in finite basis. The extrapolated r_n and r_m in Ref. [65] are larger than the values we obtained for $N_{\max} = 16$ and $N_{\max} = 18$ (Table IV). Since our r_n and r_m have an increasing trend with increasing N_{\max} around the region with the least $\hbar\Omega$ dependence, it appears reasonable that we would obtain a higher value of $r_{n/m}$ after extrapolation.

We view this work as the first step in a series of efforts we intend to make to reveal the spatial structure of exotic nuclei using *ab initio* calculation results. Since our nuclear structure studies are non-relativistic, one may foresee *ab initio* calculations that fuel driven semi-classical models capable of presenting detailed structural information of a nucleus with intuitive appeal. We will illustrate this in our future works.

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Appendix A: Harmonic oscillator matrix elements

One can obtain the matrix elements of operators $O(r) = r^0$ and $O(r) = r^2$ in the convenient HO basis with the knowledge that the angular parts of the wavefunctions are not affected, so only matrix elements with $l = l'$ are non-zero:

$$\langle n'l'|r^0|nl\rangle = \delta_{n,n'}\delta_{l,l'}, \quad (\text{A1})$$

$$\begin{aligned} & \langle n'l'|r^2|nl\rangle \\ &= b^2 \left[\left(2n+l+\frac{3}{2}\right)\delta_{n,n'} - \sqrt{n(n+l+\frac{1}{2})}\delta_{n,n'+1} \right. \\ & \quad \left. - \sqrt{(n+1)(n+l+\frac{3}{2})}\delta_{n,n'-1} \right] \delta_{l,l'}, \end{aligned} \quad (\text{A2})$$

where $b \equiv \sqrt{\hbar/(\mu\Omega)}$ with the reduced mass $\mu = m_N/2$ ($m_N = 938.92 \text{ MeV}/c^2$ is the average mass of a neutron

and a proton with their mass given by PDG [56]) representing the reduced mass of a nucleon in the two-body subsystem. The derivation of these matrix elements has been detailed in the Appendix of Ref. [66].

Appendix B: Moshinsky transformation

We follow the Moshinsky transformation as discussed in Ref. [67]. The single particle HO wave functions in the two-body relative frame are

$$\langle \vec{r}|nlm\rangle. \quad (\text{B1})$$

The two-body oscillator wave function with total angular momentum L and its projection λ reads

$$\begin{aligned} & \langle \vec{r}_1\vec{r}_2|n_1l_1n_2l_2L\lambda\rangle \\ &= R_{n_1l_1}(r_1)R_{n_2l_2}(r_2) \sum_{m_1m_2} C_{m_1m_2\lambda}^{l_1l_2L} Y_{l_1m_1}(\mathbf{\Omega}_1)Y_{l_2m_2}(\mathbf{\Omega}_2). \end{aligned} \quad (\text{B2})$$

Noting that the two-body relative coordinates

$$\vec{r} = \frac{1}{\sqrt{2}}(\vec{r}_1 - \vec{r}_2), \quad \vec{R} = \frac{1}{\sqrt{2}}(\vec{r}_1 + \vec{r}_2), \quad (\text{B3})$$

and introducing the two-body center-of-mass orbital angular momentum \mathcal{L} and its projection \mathcal{M} , and the center-of-mass radial quantum number \mathcal{N} , one arrives at

$$\begin{aligned} \langle \vec{r}\vec{R}|n_1l_1n_2l_2L\lambda\rangle &= \sum_{i\mathcal{L}} \psi_i(r, R) \\ & \quad \times \sum_{m\mathcal{M}} C_{m\mathcal{M}\lambda}^{l\mathcal{L}L} Y_{lm}(\mathbf{\Omega}_r)Y_{\mathcal{L}\mathcal{M}}(\mathbf{\Omega}_R), \end{aligned} \quad (\text{B4})$$

where $i \equiv \{n_1l_1n_2l_2L\mathcal{L}\}$, and

$$\psi_i(r, R) = \sum_{n\mathcal{N}} (nl, \mathcal{N}\mathcal{L}; L|n_1l_1, n_2l_2; L)_1 R_{ni}(r)R_{\mathcal{N}\mathcal{L}}(R), \quad (\text{B5})$$

with the well-known Moshinsky brackets $(nl, \mathcal{N}\mathcal{L}; L|n_1l_1, n_2l_2; L)_1$ subscripted by the ratio of the mass of the two bodies (see e.g. Ref. [68]).

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